

201-14936A

**HPV Assessment Report and Test Plan for  
Sodium Lauryl Sulfoacetate (Acetic Acid, sulfo-,1-dodecyl  
ester sodium salt) CAS 1847-58-1**

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18 December 2003

Prepared for STEPAN Company, Northfield, IL  
by NOTOX Safety and Environmental Research BV  
for submission under the US-HPV Challenge Program

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## 1. Introduction

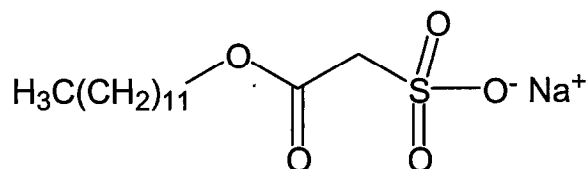
Under agreement with Stepan Company, NOTOX Safety and Environmental Research B.V. conducted an evaluation and assessment of the detergent sodium lauryl sulfoacetate (CAS 1847-58-1; commercial name: Lathanol LAL), classified as a high production volume (HPV) chemical according to criteria established by the US-EPA, i.e., >1,000,000 pounds manufactured or imported into the USA annually. Stepan Company has voluntarily agreed to complete a hazard characterization of this substance following US EPA guidance and according to the SIDS data requirements.

### Sodium lauryl sulfoacetate

CAS No. 1847-58-1

Formula:  $C_{14}H_{27}O_5SNa$

Molecular weight: 330



US EPA has identified 2800 HPV chemicals to be evaluated in the HPV Challenge Program. Sodium lauryl sulfoacetate, which is under evaluation in the present document, is listed as an HPV chemical. Sodium lauryl sulfoacetate is used as a cosmetic ingredient in personal care products. The commercial product Lathanol LAL Powder contains 64-85% active ingredient. The remaining components are sodium sulfate and sodium chloride. NOTOX has assisted Stepan Company to determine the suitability of the available data on sodium lauryl sulfoacetate to fulfill a screening level hazard characterization.

For the development of screening level health and environmental assessment information, NOTOX followed a step-wise approach incorporating the following elements:

1. a comprehensive literature search and retrieval of HPV data using the complementary CIS (Chemical Information Systems) and EU (European Union) data sources.
2. the application of computer models (SAR's) for estimating physicochemical and ecotoxicological properties of the candidate HPV substance.
3. the reviewing of studies and preparation of robust summaries
4. determination of the suitability of studies for meeting the SIDS data requirements and construction of a SIDS data matrix and recommendations for the draft testing plan.

The following is a summary of the studies available, an identification of data-gaps and recommended test plan.

## 2. Evaluation of SIDS Endpoints

An evaluation of data available on SIDS endpoints for sodium lauryl sulfoacetate is presented as follows. The robust summaries of the studies/reports evaluated (including skin/eye irritation) are contained in Appendix A.

### 2.1. Physicochemical Data

Data on all physicochemical endpoints are available and adequate for the purposes of the HPV challenge. The EPIWIN calculations performed (results in Appendix B) have their restrictions due to the fact that the salt is calculated with a covalent bond between the sodium ion and the sulfonate ion. This is considered acceptable. EPIWIN is expected to underestimate the water solubility and, therefore, overestimate the octanol-water partition coefficient. The physical form of sodium lauryl sulfoacetate is that of a powder or flake which dissolves in water. The water solubility value from the literature and the model estimate differ significantly. This is attributable to the fact that the observed solubility in the literature is probably a micellar solution and not a true solution, while the EPIWIN does not account for the formation of micellar solutions. The water solubility from the literature is taken as the key end point, because it will resemble the actual behavior of the substance when introduced in water. This was confirmed by the aquatic toxicity tests conducted at concentrations up to 100 mg/L.

Based on these considerations and values mentioned in Table 1, it is concluded that all SIDS endpoints have been adequately investigated and no further testing is recommended.

**Table 1. Physicochemical Properties**

Sodium lauryl sulfoacetate CAS 1847-58-1				
	Value	Comment	KI	Ref
Melting point (°C)	271	calculated	2	18
Boiling point (°C)	425	calculated	2	18
Relative density	0.55	review	2	9
Vapor pressure (hPa)	3.0E-14	calculated	2	18
Partition coefficient	2.66	calculated	2	18
Water Solubility (mg/L) at 25°C	10,000	review	2	9
	3.83	calculated	2	18
Dissociation constant	-0.5	calculated	1	10

KI = Klimisch criteria

Ref = Reference number

### 2.2. Environmental Fate

Table 2 presents a summary of available data. Data on all SIDS endpoints are available and adequate. The photodegradation in air represented by the Atmospheric Oxidation Potential or AOP model was calculated by EPIWIN to be 7.9 hours. Sodium lauryl sulfoacetate is reported as stable in water in a pH range of 5.0 to 8.5 (9). Calculation of the environmental distribution (Fugacity) at Mackay level III with discharge of the substance into water, showed that > 99% of the substance will stay in the water and that a small percentage goes to sediment.

In a biodegradation study following the OECD 301B guideline the test substance did not meet the criteria for ready biodegradability (>60% within a 10-d period) but was shown to be biodegradable to a major extent (56% removal in 29 days). Biodegradation would be considered a pathway for the removal of this substance in the environment

Based on this evaluation and data, all endpoints for environmental fate have been sufficiently investigated and the data is considered reliable and adequate. No further testing of these properties is recommended.

**Table 2. Environmental Fate Properties**

Sodium lauryl sulfoacetate CAS 1847-58-1				
	Value	Comment	KI	Ref
Photodegradation (t1/2 hrs)	7.9	calculated	4	18
Hydrolysis	Stable	review	4	9
Transport between compartments (% in water/air/soil/sediment)	99.3/0/0/0.65		2	18
Ready Biodegradability	not readily biodegradable	56% in 29 days; OECD 301B	1	11

KI = Klimisch criteria

Ref = Reference number

### 2.3. Ecotoxicity

Table 3 presents a summary of available data. Reliable and adequate data are available on the daphnia acute toxicity and algal inhibition endpoints. Freshwater algae were the most sensitive species tested. The actual concentration/effect relationship (mg/L) measured for both daphnia and algae confirmed the values estimated by the ECOSAR model. Based on the comparable data shown in Table 3, it is expected that acute fish toxicity will also fall into a similar mg/L concentration range. Because two reliable studies with measured concentrations are available to establish acute aquatic effects and these values confirm the modelling estimates it is not considered necessary to determine acute fish toxicity.

Based on the information available, acute effects on representative aquatic organisms have been sufficiently investigated and considered adequate for the HPV challenge program. The substance is considered moderately toxic to aquatic organisms.

**Table 3. Ecotoxicity**

Sodium lauryl sulfoacetate CAS 1847-58-1				
	Value	Comment	KI	Ref
Fish (96 h-LC50; mg/L)	22.2	calculated (ester)	4	18
Daphnia (48 h-LC50; mg/L)	5.9	OECD 202	1	13
	65.8	calculated (ester)	4	18
Algae (72 h-EC50; mg/L)	1.9	OECD 201	1	14
EC Biomass	1.8	96 h calculated (ester)	4	18

KI = Klimisch criteria

Ref = Reference number

## 2.4. Mammalian Toxicity

The human health effects data for SIDS endpoints are presented in Table 4. An acute oral LD50 value in the rat of > 2000 mg/kg body weight and an acute dermal LD50 value in rabbit of greater than 2000 mg/kg body weight are available. In view of its use (cosmetic) the dermal route is considered to be the most appropriate for this product. Repeated dose (28-day and 90-day) toxicity studies reported a NOAEL of 200 mg/kg/day and a NOAEL of 75 mg/kg/day, respectively. In both the Ames test and chromosomal aberration study the substance was shown not to be genotoxic with or without metabolic activation.

For the non-SIDS endpoints skin and eye irritation studies following the OECD guidelines showed that sodium lauryl sulfoacetate is moderately irritating to skin and eye. In the Journal of the American College of Toxicology (Ref 9) Cosmetic Ingredient Review (CIR) the Expert Panel concluded that sodium lauryl sulfoacetate is safe as a cosmetic ingredient in the present practices of use and concentrations.

Based on the present evaluation, all human health endpoints are adequately described with the exception of reproduction/developmental toxicity.

**Table 4. Mammalian Toxicity**

Sodium lauryl sulfoacetate CAS 1847-58-1				
	Value	Comment	KI	Ref
<i>Acute Toxicity</i>				
Acute Oral (LD50; mg/kg bw)	>2000	limit test ; OECD 401	1	1
Acute Dermal (LD50; mg/kg bw)	>2000	limit test ; OECD 402	1	2
Acute inhalation (LC50; mg/m <sup>3</sup> )	-			
<i>Genetic Toxicity</i>				
Ames test	negative	with and without metab. activity; single experiments	2	6-8
Chromosomal aberration	negative	OECD 473	1	12
<i>Subchronic/Reproduction</i>				
28 day (NOAEL) (LOAEL)	200 800	limited examinations	2	4
90 day (NOAEL) (LOAEL)	75 250		1	5
Reproduction toxicity	-			
Developmental toxicity	-			

KI = Klimisch criteria

Ref = Reference number

## 3. SIDS Data Matrix

Sodium lauryl sulfoacetate CAS 1847-58-1				
	Value	Comment	KI	Ref
<b>Physicochemical data</b>				
Melting point (°C)	271		2	18
Boiling point (°C)	425		2	18
Relative density	0.55		2	9
Vapor pressure (hPa)	3 .0E-14		2	18
Partition coefficient	2.66		2	18
Water Solubility (mg/L) at 25°C	10,000		2	9
	3.83		2	18
Dissociation constant	-0.5	calculated	1	10
<b>Environmental fate</b>				
Photodegradation (t1/2 hrs)	7.9		4	18
Hydrolysis	Stable	review	4	9
Transport between compartments (% in water/air/soil/sediment)	99.3/0/0/0.65		2	18
Ready Biodegradability	not readily biodegradable	56% in 29 days; OECD 301B	1	11
<b>Ecotoxicity</b>				
Fish (96 h-LC50; mg/L)	22.2	calculated (ester)	4	18
Daphnia (48 h-LC50; mg/L)	5.9	OECD 202	1	13
	65.8	calculated (ester)	4	18
Algae (72 h-EC50; mg/L)	1.9	EC biomass; OECD 201	1	14
	1.8	96 h calculated (ester)	4	18
<b>Mammalian toxicity</b>				
<b>Acute Toxicity</b>				
Acute Oral (LD50; mg/kg)	>2000	limit test; OECD 401	1	1
Acute Dermal (LD50; mg/kg)	>2000	limit test; OECD 402	1	2
Acute inhalation (LC50; mg/m <sup>3</sup> )	-			
<b>Genetic Toxicity</b>				
Ames test	negative	with and without metab. activity; single experiments	2	6-8
Chromosomal aberration	negative	OECD 473	1	12
<b>Subchronic/Reproduction</b>				
28 day (NOAEL)	200	limited examinations	2	4
90 day (NOAEL)	75		1	5
Reproduction toxicity	NA			
Developmental toxicity	NA			

NA – data not available

#### 4. Data Availability and Testing Plan

The availability of data is depicted in the following table. The study that should be performed to fill a data gap has been indicated.

**Table 6. Testing Plan**

	<b>Sodium lauryl sulfoacetate CAS 1847-58-1</b>
<b>Physico-chemical</b>	
Melting point	+
Boiling point	+
Density	+
Vapor Pressure	+
Partition Coefficient	+
Water Solubility	+
<b>Environmental Fate</b>	
Photodegradation	+
Hydrolysis	+
Transport between compartments	+
Biodegradability	+
<b>Ecotoxicity*</b>	
96-h LC50 Fish	+
48-h EC50 Daphnia	+
72-h EC50 Algal Inhibition	+
<b>Mammalian toxicity</b>	
Acute	+
Repeated dose	+
Genetic Toxicity	+
Reproduction/developmental	<b>OECD421</b>

+ = data available and adequate

OECD = test to be performed

#### Conclusion

For the purpose of the HPV Challenge program adequate and reliable data are available on the physicochemical properties, environmental fate and ecotoxicity of sodium lauryl sulfoacetate. For mammalian toxicity endpoints, reliable and adequate data are also available for acute toxicity, genetic toxicity and repeated dose toxicity. Reproduction and developmental toxicity is not known. Therefore, a reproduction/developmental toxicity screening test following OECD Guideline 421 will be conducted to complete the hazard characterization of this substance.



## 5. References

	Author	Title	Source/performing laboratory	Year
1.	Kukulinski, M.	Acute oral study (TM study 97-119-3A)	Tox Monitor Laboratories	1997
2.	Kukulinski, M.	Acute dermal toxicity study (TM study 97-119-4)	Tox Monitor Laboratories	1997
3.	Marks, K.H.	Determination of ready biodegradability closed bottle test (Weston study 91-001)	Roy F. Weston, Fate and Effect Laboratory	1992
4.	Hill, R	28 Day oral range finding study in the rat toxicol report ref. Sus/1/c	Toxicol Laboratories Ltd	1985
5.	Hill, R	90 Day oral toxicity study in the rat 910-74	Toxicol Laboratories Ltd	1986
6.	Anonymous	No title; labelled 2-18-5	Litton Bionetics	1978
7.	Anonymous	Mutagenicity evaluation of 2300-00, lot 23N056 in the Ames Salmonella/microsome plate test.	Litton Bionetics	1978
8.	Anonymous	Mutagenicity evaluation of 3000-00, lot 30M366 in the Ames Salmonella/microsome plate test.	Litton Bionetics	1978
9.	Anonymous	Final report on the safety assessment of sodium lauryl sulfoacetate.	J. Am. Coll. Toxicol. 6(3), 261-277	1987
10.	Brekelmans, M.J.C.	Statement on the determination of the dissociation constant(s) of Lathanol LAL powder in water.	NOTOX BV	2003
11.	Desmares-Koopmans, M.J.E.	Determination of 'ready' biodegradability: carbon dioxide (CO <sub>2</sub> ) evolution test (modified Sturm test) with Lathanol LAL powder.	NOTOX BV	2003
12.	Buskens, C.A.F.	Evaluation of the ability of Lathanol LAL powder to induce chromosome aberrations in cultured peripheral human lymphocytes.	NOTOX BV	2003
13.	Bouwman, L.M.	Acute toxicity study in Daphnia magna with Lathanol LAL powder (semi-static).	NOTOX BV	2003
14.	Bouwman, L.M.	Fresh water algal growth inhibition test with Lathanol LAL powder.	NOTOX BV	2003
15.	Kukulinski, M.	OECD guideline 404 primary dermal irritation/corrosion study (TM 97-119-2)	Tox Monitor Laboratories, Inc.	1997
16.	Bankhead, R.R.	DOT Test for corrosivity.	Rosner Hixson Laboratories	1977
17.	Kukulinski, M.	OECD guideline 405 acute eye irritation/corrosion study (TM 97-119-1).	Tox Monitor Laboratories, Inc.	1997
18.		EPISUITE v3.10 (April 2001).		2001